Probing quantum statistical mechanics with Bose gases: Non-trivial order parameter topology from a Bose-Einstein quench

J.R. Anglin[a,b] and W.H. Zurek[b]

[a]Institut für Theoretische Physik, Universität Innsbruck, Austria

[b]T-6, MS B288, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

A rapid second order phase transition can have a significant probability of producing a metastable state instead of the equilibrium state. We consider the case of rapid Bose-Einstein condensation in a toroidal trap resulting in a spontaneous superfluid current, and compare the phenomenological time-dependent Ginzburg-Landau theory with quantum kinetic theory. A simple model suggests the effect should be observable.

1. THE ORDER PARAMETER AND THE EFFECTIVE POTENTIAL

A qualitative understanding of a second order phase transition may be had by considering the system to be described by a two-component *order parameter*, consisting of a modulus R and an angle θ[1]. The order parameter is taken to behave as a particle in a two-dimensional effective potential $V(R)$, with some form of dissipation dragging the system towards the bottom of this potential (possibly opposed by some random noise).

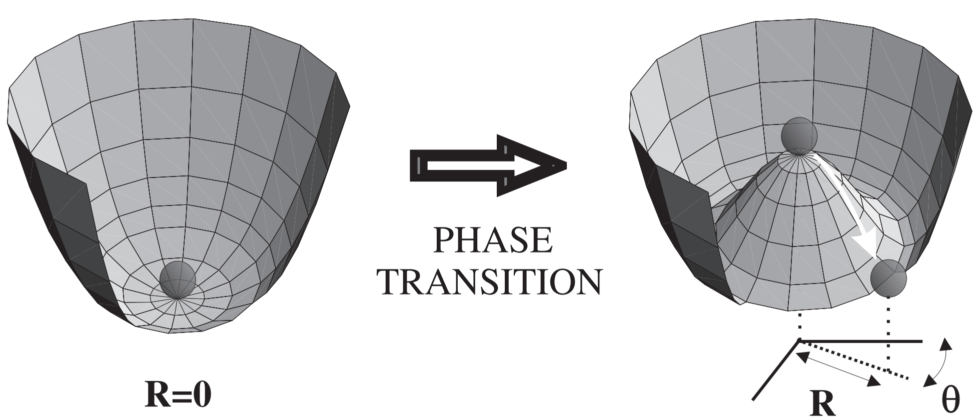

Figure 1: Effective potential theory of a second order transition.

In the disordered phase of the system, the minimum of $V(R)$ is at $R = 0$, so that θ is indefinite (or purely random) (Fig. 1, left picture). The phase transition then occurs

through a modification of the effective potential, such that $R = 0$ becomes a local maximum, and the new minimum is a circular trough at some finite radius. The system rolls down the central hill to the trough, (Fig. 1, right picture) and θ acquires a definite value (with only small fluctuations due to noise). Which definite value θ acquires, however, is random, determined by small fluctuations while the system is near $R = 0$.

One can also allow R, θ to be functions of position (with $V(R)$ assumed to have the same form everywhere). In the ordered phase, the definite angle $\theta(x)$ may then vary spatially. A qualitative question thus arises, namely the topology of $\theta(x)$. Suppose we let x lie on a circle, for example: what *winding number* $\oint dx\, \partial_x\theta/(2\pi)$ should we typically observe after a transition? If the transition is slow, $\theta(x)$ will have time to organize itself all around the circle into some lowest energy configuration (such as $\theta(x)$ constant); but if it is fast, the random choice of θ around the circle will have some finite correlation length, and non-zero winding number will sometimes result. If it does, it will tend to be stable, since there is a high effective potential barrier for $R = 0$, and without making $R(x) \to 0$ somewhere, it is impossible to alter the winding number. See Fig. 2.

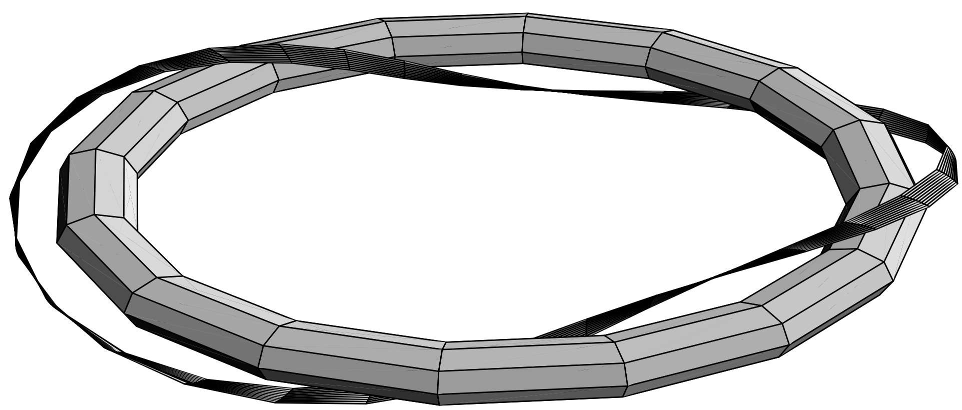

Figure 2: Winding number two; distance of ribbon from torus represents $R(x)$, angle of winding around torus represents $\theta(x)$.

The emergence of non-trivial topology from a rapid (quench-like) phase transition is common to a wide range of physical systems, real and postulated, from vortex loops in superfluid helium[2,3] to cosmic strings in the early universe[4,2]. With the advent of dilute alkali gas Bose condensates[5], we can now investigate this basic statistical mechanical problem in a new arena. The condensate mean field wave function $\psi = Re^{i\theta}$ provides our order parameter; and the current experimental technique of evaporative cooling automatically provides a rapid phase transition (on the Boltzmann scattering time scale). Our example of x lying on a circle can realistically be achieved with a toroidal trap, sufficiently tight for the system to be approximately one-dimensional. (We will consider such a trap of circumference $\sim 100\mu$m, which we understand is a credible prospect for the relatively near future.) In this context, non-zero winding number implies circulation around the trap, since $\nabla\theta$ is the superfluid velocity. (Angular momentum conservation is an issue we will discuss briefly below, only noting for now that the condensate is not isolated.)

2. TIME-DEPENDENT GINZBURG-LANDAU THEORY

To proceed to a quantitative description of our subject, we first consider the phenomenological theory obtained by letting the time evolution of ψ be governed by a first order equation involving a potential of the Ginzburg-Landau form we have sketched above:

$$\tau_0 \dot{\psi} = \beta \Big(\frac{\hbar^2}{2M} \nabla^2 + \mu - \Lambda |\psi|^2 \Big) \psi \ , \tag{1}$$

where $\beta = (k_B T)^{-1}$, and τ_0 and $\Lambda > 0$ are phenomenological parameters. The thermodynamical variable μ behaves near the critical point, in the case we consider, as

$$\mu = \frac{3}{2}(T_c - T) + \mathcal{O}(T_c - T)^2 \ , \tag{2}$$

where T_c is the critical temperature. The equilibration time for long wavelengths is $\tau = \tau_0 k_B T / |\mu|$. The system's disordered phase is described by $\mu < 0$; the ordered phase appears when $\mu > 0$. Note that this time-dependent Ginzburg-Landau (TDGL) theory also typically assumes some small stochastic forces acting on ψ; we will leave these implicit.

A quench occurs if μ changes with time from negative to positive values. The divergence of the equilibration time τ at the critical point $\mu = 0$ is associated with *critical slowing down*. Because of this critical slowing down, $\frac{d\mu}{dt}/\mu$ must exceed $1/\tau$ in some neighbourhood of the critical point, and so there must be an epoch in which the system is out of equilibrium. What are at the beginning of this epoch mere fluctuations in the disordered phase, in which higher energy modes happen momentarily to be more populated than the lowest mode, can thus pass unsuppressed by equilibration into the ordered phase, to become topologically non-trivial configurations of $\psi(x)$.

The interval within which equilibration is negligible can be identified as the period wherein $|t|/\tau < 1$. If we define the quench time scale τ_Q by letting $\beta\mu = t/\tau_Q$ (choosing $t = 0$ as the moment the system crosses the critical point), this implies that the crucial interval is $-\hat{t} < t < \hat{t}$, for $\hat{t} = \sqrt{\tau_Q \tau_0}$. The correlation length $\hat{\xi}$ for fluctuations at time $t = -\hat{t}$ is then given by $\hbar/(2M\hat{\xi}^2) = \mu(-\hat{t})$, which (assuming $T(-\hat{t}) \doteq T_c$) implies that $\hat{\xi} = \lambda_{T_c} (\tau_Q/\tau_0)^{1/4}$, for $\lambda_T = \hbar (2 M k_B T)^{-\frac{1}{2}}$ the thermal de Broglie wavelength[2]. Assuming one independently chosen phase within each correlation length $\hat{\xi}$, then modeling the phase distribution around the torus as a random walk suggests that the net winding number should be of order $\sqrt{L/\hat{\xi}}$ for L the trap circumference. Since evaporative cooling may be expected to yield $(\tau_Q/\tau_0)^{1/4}$ of order one, and T_c is several hundred nK, we can estimate $\hat{\xi} \sim 100$ nm, leading us to expect winding numbers in our 100μm torus of order ten. At current experimental densities, this implies a current approaching the Landau critical velocity, in the range of mm/s.

Considering this intriguing possibility raises an obvious question: is TDGL actually relevant to finite samples of dilute gas, far from equilibrium?

3. QUANTUM KINETIC THEORY

Because the condensates now available are dilute enough to be weakly interacting, there are good prospects for answering this question theoretically, by constructing from

first principles a quantum kinetic theory to describe the whole process accurately. Using a second-quantized description of the trapped gas, one treats all modes above some judiciously chosen energy level as a reservoir of particles, coupled to the lower modes by two-particle scattering. Tracing over the reservoir modes leads to a master equation for the low energy modes[6], very similar to the equation for a multimode laser. Scattering of particles from the reservoir modes into the low modes, and vice versa, provides gain and loss terms. If the reservoir is described at all times by a grand canonical ensemble (of time-dependent temperature and chemical potential, in general), then the gain and loss processes are related by a type of fluctuation-dissipation relation, in which the reservoir chemical potential and the repulsive self-interaction of the gas combine in precisely the Ginzburg-Landau form. As a result, as long as these gain and loss processes are the only significant scattering channels, and the condensate self-Hamiltonian can be linearized to a good approximation, the system is indeed described quite well by time-dependent Ginzburg-Landau theory. Since these two conditions can be shown to hold near the critical point, all the results of section 2 can be recovered from quantum kinetic theory.

We can also clarify how the onset of a runaway process like Bose-Einstein condensation by evaporation can be consistent with critical slowing down: though the particle numbers in the lowest modes of the trapped gas are growing very fast, the required particle numbers to be in equilibrium with the higher energy modes grow much faster still as the temperature passes through T_c. So even with Bose-enhanced scattering at ever increasing rates, the rate at which the system is able to maintain equilibrium actually decreases.

The problem is that circulating states only become metastable above a threshold density, precisely because nonlinearity is required. So understanding the probability for a circulating condensate to grow into metastability requires extending quantum kinetic theory into the fully nonlinear regime, and without begging the basic question by assuming from the start that some particular mode will end up with the condensate.

3.1. A two-mode model

As a first step towards this goal, we consider a toy model of just two competing modes, such as the torus modes of different winding numbers k_0, k_1. The self-Hamiltonian of this system is taken as

$$\hat{H} = E[\hat{n}_1 + \frac{1}{2N_c}(\hat{n}_0^2 + \hat{n}_1^2 + 4\hat{n}_1\hat{n}_0)] \,. \tag{3}$$

Since the self-Hamiltonian must conserve both particle number and angular momentum, it can only be a function of $\hat{n}_0$ and $\hat{n}_1$ (which greatly simplifies the derivation of the master equation). Because we have incorporated the Bose enhancement of inter-mode repulsion (the factor of 4 instead of 2 in front of the $\hat{n}_0\hat{n}_1$ term, which is of course the best case value, obtained when the two orbitals overlap completely), we make the state with all particles in the 1 mode a local minimum of the energy for fixed $n_0 + n_1 > (N_c + 1)$. We have thus obtained an simple model which exhibits metastability above a threshold.

To make our results more meaningful, we estimate the experimental ranges of our parameters E and N_c. For our toroidal trap βE would be on the order of 10^{-4} at current experimental temperatures, and proportional to $k_1^2 - k_0^2$. N_c would be of order one for $(k_0, k_1) = (0, 1)$, but higher for higher modes (since E/N_c is actually constant).

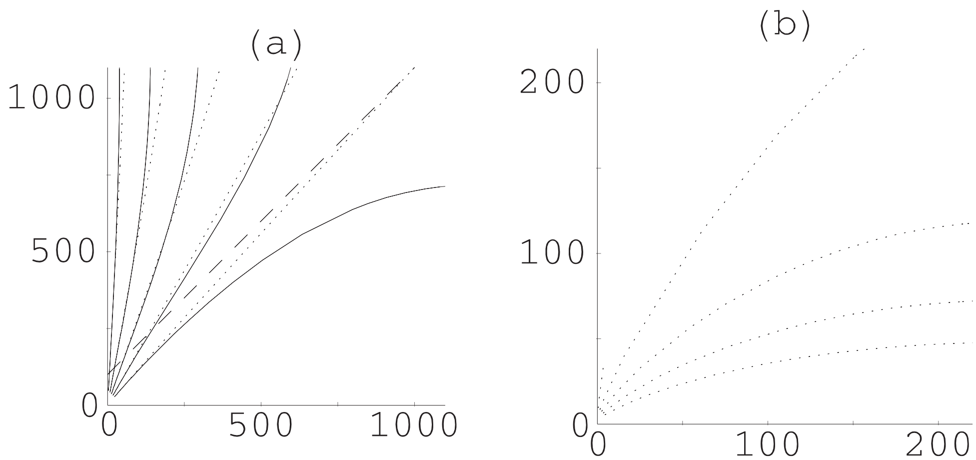

Figure 3: Trajectories from QKT (solid) and TDGL (dotted); heavy dashed line is threshold for metastability of mode 1. Initial times are $\hat{t}$; quench is $\beta\mu = \tanh(t/\tau_Q)$, $\beta = \beta_c e^{\tanh(t/\tau_Q)}$. Parameters are $N_c = 100$, and (a) $\Gamma\tau_Q = 10$, $\beta_c E = 0.01$; (b) $\Gamma\tau_Q = 100$, $\beta_c E = 0.05$. All trajectories shown initially have $n_1 > n_0$.

Tracing out a reservoir of higher modes as described above leads to a master equation for the two modes 0 and 1, which even for this highly simplified model is only directly tractable numerically. Here we will simply consider it as a kind of Fokker-Plank equation for the particle numbers n_0, n_1, and by neglecting the diffusion terms (valid for fast quenches after the early stage, which can be solved separately by assuming linearity), we extract an equation of motion for n_0 and n_1 which we can compare to TDGL:

$$\begin{aligned}
\dot{n}_0 &= \Gamma n_0 \Big[e^{\beta\mu} - e^{\frac{\beta E}{N_c}(n_0+2n_1)} + 2\beta E n_1 e^{-\frac{\beta E}{2N_c}|N_c+n_0-n_1|} \sinh \frac{\beta E}{2N_c}(N_c+n_0-n_1) \Big] \\
\dot{n}_1 &= \Gamma n_1 \Big[e^{\beta\mu} - e^{\frac{\beta E}{N_c}(N_c+n_1+2n_0)} - 2\beta E n_0 e^{-\frac{\beta E}{2N_c}|N_c+n_0-n_1|} \sinh \frac{\beta E}{2N_c}(N_c+n_0-n_1) \Big].
\end{aligned}$$

When $n_0 + 2n_1$ and $N_c + n_1 + 2n_0$ are both close to $N_c\mu/E$, or for low enough particle numbers, we may replace $n_j \to |\psi_j|^2$ in the first two terms in each equation of (3) to obtain a TDGL equation, in the sense that $\dot{\psi}_j$ is set equal to the variation of a Ginzburg-Landau effective potential with respect to ψ_j^*. But the last term in each equation is not of Ginzburg-Landau form (it does not even involve μ). These non-GL terms conserve $n_0 + n_1$, and so are neither gain nor loss but another scattering channel hitherto neglected: collisions with reservoir particles shifting particles between our two low modes. These processes are insignificant at low particle numbers, but grow much stronger as the condensate grows larger, because they are doubly Bose-enhanced. And they turn out to have a simple but potentially drastic effect: they allow they system to equilibrate in energy faster than in particle number.

Representative solutions to (3) are shown in Fig. 3, together with the $|\psi_j|^2$ given by the TDGL theory formed by keeping only the first two terms of each equation in (3), expanding the exponentials to first order. It is clear that for sufficiently fast quenches the two theories accord quite well, but that for slower quenches TDGL significantly overestimates the probability of reaching the metastable state, because more rapid equilibration

in energy than particle number strongly favours the lowest mode. This is the main new feature we have identified in dilute Bose gases as a GL-like system.

3.2. Angular momentum

Finally, we return to the question of angular momentum. Spontaneous appearance of a circulating state, condensing out of a cold atomic cloud with no net rotation, obviously implies angular momentum concentration in the condensate. Compensating ejection of fast atoms with opposite angular momentum during the evaporation process, in which after all most of the initial atoms are expelled, is a plausible mechanism by which this can proceed. Our assumption that the non-condensate atoms remain in a grand canonical ensemble relies implicitly on some such process. In our two-mode model, constraining the reservoir's mean angular momentum to be always opposite to that of the condensate will effectively just raise E and N_c. Angular momentum transport during evaporative cooling has as yet received no detailed study, however.

4. CONCLUSIONS

Despite the shortcomings of TDGL revealed by our toy model, we emphasize that kinetic theory does show that TDGL is indeed relevant to trapped dilute gases: what TDGL requires is not outright rejection, but corrections. And although the corrections may be substantial, the qualitative features predicted by TDGL are still recovered. While the extension of quantum kinetic theory beyond toy models, to realistic descriptions of spontaneous currents, will obviously require further study, the prospects for experimental realization of spontaneous currents are quite encouraging. Athough in this brief treatment we have neglected noise, diffusive nucleation actually gives a lower bound of typical winding number one for condensation in our hundred micron toroidal trap; with 10^6 atoms, even this has an equilibrium probability of order e^{-10}.

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